Lan Cheng

List of Publications by Year
in descending order

58 papers	1,787 citations	331670 21 h-index	276875 41 g-index
58 all docs	58 docs citations	58 times ranked	1476 citing authors

#	Article	IF	Citations
1	Spectroscopy on the electron-electric-dipole-momentâ€“sensitive states of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi mathvariant="normal">ThF</mml:mi><mml:mo>+</mml:mo></mml:msup></mml:math>. Physical Review A, 2022, 105, .	2.5	7
2	Quadratic Unitary Coupled-Cluster Singles and Doubles Scheme: Efficient Implementation, Benchmark Study, and Formulation of an Extended Version. Journal of Chemical Theory and Computation, 2022, 18, 2281-2291.	5.3	4
3	Geometry optimizations with spinor-based relativistic coupled-cluster theory. Journal of Chemical Physics, 2022, 156, 151101.	3.0	5
4	Inner-shell excitation in the YbF molecule and its impact on laser cooling. Journal of Molecular Spectroscopy, 2022, 386, 111625.	1.2	8
5	Photoelectron spectroscopy of cryogenically cooled NiO₂^{â^’}via slow photoelectron velocity-map imaging. Physical Chemistry Chemical Physics, 2022, 24, 17496-17503.	2.8	2
6	Atomic Mean-Field Approach within Exact Two-Component Theory Based on the Diracâ€“Coulombâ€“Breit Hamiltonian. Journal of Physical Chemistry A, 2022, 126, 4537-4553.	2.5	15
7	Analytic evaluation of energy first derivatives for spinâ€“orbit coupled-cluster singles and doubles augmented with noniterative triples method: General formulation and an implementation for first-order properties. Journal of Chemical Physics, 2021, 154, 064110.	3.0	11
8	Photoelectron Spectroscopic and ab Initio Computational Studies of the Anion, HThO^{â€“}. Journal of Physical Chemistry A, 2021, 125, 1903-1909.	2.5	2
9	Relativistic coupledâ€cluster and equationâ€ofâ€motion coupledâ€cluster methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1536.	14.6	26
10	Anion photoelectron spectroscopic and relativistic coupled-cluster studies of uranyl dichloride anion, UO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e792" altimg="si74.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>Cl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e800" altimg="si76.svg"><mml:msubsup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml:	1.2	3
11	Calculations of time-reversal-symmetry-violation sensitivity parameters based on analytic relativistic coupled-cluster gradient theory. Physical Review A, 2021, 104, .	2.5	10
12	Electronic structure of NdO via slow photoelectron velocity-map imaging spectroscopy of NdO---. Journal of Chemical Physics, 2021, 155, 114305.	3.0	4
13	Multiphoton Control of 6ÏŒ Photocyclization via State-Dependent Reactantâ€“Product Correlations. Journal of Physical Chemistry Letters, 2021, 12, 9493-9500.	4.6	3
14	Limitations of perturbative coupled-cluster approximations for highly accurate investigations of Rb2+. Journal of Chemical Physics, 2021, 155, 124101.	3.0	1
15	Accurate prediction and measurement of vibronic branching ratios for laser cooling linear polyatomic molecules. Journal of Chemical Physics, 2021, 155, 091101.	3.0	30
16	Unitary coupled-cluster based self-consistent polarization propagator theory: A quadratic unitary coupled-cluster singles and doubles scheme. Journal of Chemical Physics, 2021, 155, 174102.	3.0	5
17	Towards accurate prediction for laser-coolable molecules: relativistic coupled-cluster calculations for yttrium monoxide and prospects for improving its laser cooling efficiencies. Physical Chemistry Chemical Physics, 2020, 22, 26167-26177.	2.8	10
18	Mapping the Electronic Structure of the Uranium(VI) Dinitride Molecule, UN2. Journal of Physical Chemistry A, 2020, 124, 6486-6492.	2.5	8

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19	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	3.0	375
20	Branching Ratios, Radiative Lifetimes, and Transition Dipole Moments for YbOH. Journal of Physical Chemistry A, 2020, 124, 3135-3148.	2.5	20
21	Hetero-site Double Core Ionization Energies with Sub-electronvolt Accuracy from Delta-Coupled-Cluster Calculations. Journal of Physical Chemistry A, 2020, 124, 4413-4426.	2.5	11
22	Performance of an atomic mean-field spinâ€“orbit approach within exact two-component theory for perturbative treatment of spinâ€“orbit coupling. Molecular Physics, 2020, 118, e1768313.	1.7	15
23	Coupled cluster study of the x-ray absorption spectra of formaldehyde derivatives at the oxygen, carbon, and fluorine K-edges. Journal of Chemical Physics, 2019, 151, 064107.	3.0	24
24	Performance of Delta-Coupled-Cluster Methods for Calculations of Core-Ionization Energies of First-Row Elements. Journal of Chemical Theory and Computation, 2019, 15, 4945-4955.	5.3	50
25	A study of non-iterative triples contributions in relativistic equation-of-motion coupled-cluster calculations using an exact two-component Hamiltonian with atomic mean-field spin-orbit integrals: Application to uranyl and other heavy-element compounds. Journal of Chemical Physics, 2019, 151, 104103.	3.0	14
26	Benchmark Calculations of K-Edge Ionization Energies for First-Row Elements Using Scalar-Relativistic Coreâ€“Valence-Separated Equation-of-Motion Coupled-Cluster Methods. Journal of Chemical Theory and Computation, 2019, 15, 1642-1651.	5.3	54
27	Optical Stark and Zeeman Spectroscopy of Thorium Fluoride (ThF) and Thorium Chloride (ThCl). Journal of Physical Chemistry A, 2019, 123, 1423-1433.	2.5	6
28	Visible and ultraviolet laser spectroscopy of ThF. Journal of Molecular Spectroscopy, 2019, 358, 1-16.	1.2	8
29	Exact two-component equation-of-motion coupled-cluster singles and doubles method using atomic mean-field spin-orbit integrals. Journal of Chemical Physics, 2019, 150, 074102.	3.0	32
30	An analysis of the performance of coupled cluster methods for K-edge core excitations and ionizations using standard basis sets. Advances in Quantum Chemistry, 2019, 79, 241-261.	0.8	30
31	A theoretical and experimental benchmark study of core-excited states in nitrogen. Journal of Chemical Physics, 2018, 148, 064106.	3.0	27
32	Perturbative treatment of spin-orbit-coupling within spin-free exact two-component theory using equation-of-motion coupled-cluster methods. Journal of Chemical Physics, 2018, 148, 044108.	3.0	40
33	Two-component relativistic coupled-cluster methods using mean-field spin-orbit integrals. Journal of Chemical Physics, 2018, 148, 034106.	3.0	42
34	Matrix-Isolation and Quantum-Chemical Analysis of the C3v Conformer of XeF6, XeOF4, and Their Acetonitrile Adducts. Journal of Physical Chemistry A, 2018, 122, 119-129.	2.5	17
35	Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications. Journal of Chemical Physics, 2018, 148, 244110.	3.0	27
36	An atomic mean-field spin-orbit approach within exact two-component theory for a non-perturbative treatment of spin-orbit coupling. Journal of Chemical Physics, 2018, 148, 144108.	3.0	58

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37	Bond Dissociation Energies for Diatomic Molecules Containing 3d Transition Metals: Benchmark Scalar-Relativistic Coupled-Cluster Calculations for 20 Molecules. Journal of Chemical Theory and Computation, 2017, 13, 1044-1056.	5.3	81
38	The electric dipole moments in the ground states of gold oxide, AuO, and gold sulfide, AuS. Journal of Chemical Physics, 2017, 146, 064307.	3.0	7
39	Low-lying vibronic level structure of the ground state of the methoxy radical: Slow electron velocity-map imaging (SEVI) spectra and KÃ¶ppel-Domcke-Cederbaum (KDC) vibronic Hamiltonian calculations. Journal of Chemical Physics, 2017, 146, 224309.	3.0	15
40	Characterization of the [18.28]0â^'â€“a3Î"1 (0,0) band of tantalum nitride, TaN. Journal of Chemical Physics, 2017, 147, 154304.	3.0	0
41	Benchmark calculations on the nuclear quadrupole-coupling parameters for open-shell molecules using non-relativistic and scalar-relativistic coupled-cluster methods. Journal of Chemical Physics, 2015, 143, 064301.	3.0	1
42	Relativistic coupled-cluster calculations on XeF6: Delicate interplay between electron-correlation and basis-set effects. Journal of Chemical Physics, 2015, 142, 224309.	3.0	13
43	Inner-shell photoionization and core-hole decay of Xe and XeF2. Journal of Chemical Physics, 2015, 142, 224302.	3.0	15
44	The permanent electric dipole moment of gold chloride, AuCl. Molecular Physics, 2015, 113, 2073-2080.	1.7	3
45	Analytic energy derivatives in relativistic quantum chemistry. International Journal of Quantum Chemistry, 2014, 114, 1108-1127.	2.0	35
46	Perturbative treatment of spin-orbit coupling within spin-free exact two-component theory. Journal of Chemical Physics, 2014, 141, 164107.	3.0	27
47	Spin-free Dirac-Coulomb calculations augmented with a perturbative treatment of spin-orbit effects at the Hartree-Fock level. Journal of Chemical Physics, 2013, 139, 214114.	3.0	15
48	The Simplest Criegee Intermediate (H₂Câ•Oâ€“O): Isotopic Spectroscopy, Equilibrium Structure, and Possible Formation from Atmospheric Lightning. Journal of Physical Chemistry Letters, 2013, 4, 4133-4139.	4.6	88
49	The bromine nuclear quadrupole moment revisited. Molecular Physics, 2013, 111, 1382-1389.	1.7	7
50	Rotational spectra of rare isotopic species of fluoroiodomethane: Determination of the equilibrium structure from rotational spectroscopy and quantum-chemical calculations. Journal of Chemical Physics, 2012, 137, 024310.	3.0	24
51	The route to high accuracy in ab initio calculations of Cu quadrupole-coupling constants. Journal of Chemical Physics, 2012, 137, 224302.	3.0	17
52	Analytical evaluation of first-order electrical properties based on the spin-free Dirac-Coulomb Hamiltonian. Journal of Chemical Physics, 2011, 134, 244112.	3.0	42
53	Analytic energy gradients for the spin-free exact two-component theory using an exact block diagonalization for the one-electron Dirac Hamiltonian. Journal of Chemical Physics, 2011, 135, 084114.	3.0	136
54	Direct perturbation theory in terms of energy derivatives: Scalar-relativistic treatment up to sixth order. Journal of Chemical Physics, 2011, 135, 194114.	3.0	10

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55	Analytic second derivatives for the spin-free exact two-component theory. Journal of Chemical Physics, 2011, 135, 244104.	3.0	35
56	Making four- and two-component relativistic density functional methods fully equivalent based on the idea of â€œfrom atoms to moleculeâ€• Journal of Chemical Physics, 2007, 127, 104106.	3.0	210
57	Introduction to the John Stanton special issue. Molecular Physics, 0, , .	1.7	0
58	Benchmark Relativistic Delta-Coupled-Cluster Calculations of K-Edge Core-Ionization Energies for Third-Row Elements. Physical Chemistry Chemical Physics, 0, , .	2.8	2